Thermo-Kinetic Model of Burning for Polymeric Materials

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Key Long-Term Objectives

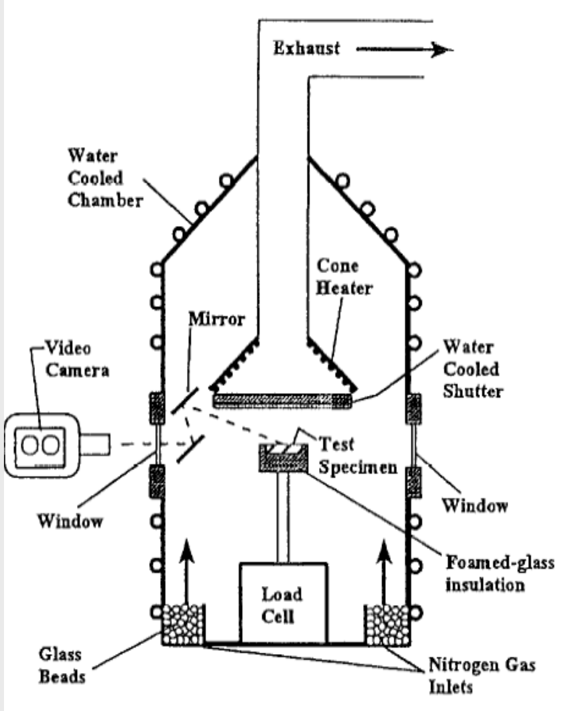
- ❑ Develop a versatile model for simulation of bench-scale flammability tests.
- ❑ Parameterize this model for various types of polymeric materials.
- ❑ Relate parameters (properties) used in the model to molecular structure.

Flammability Measurement Techniques

Cone Calorimetry
(heat release measurement)

Fire Propagation Apparatus
(heat release measurement)

Gasification Apparatus
(mass loss measurement)



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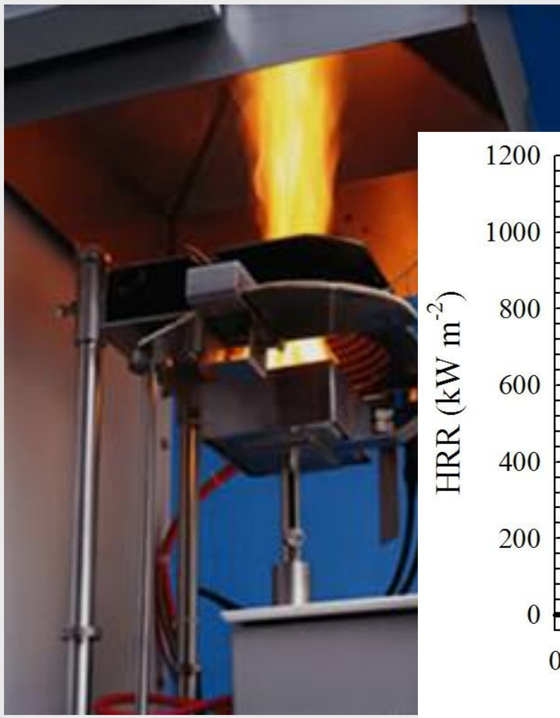
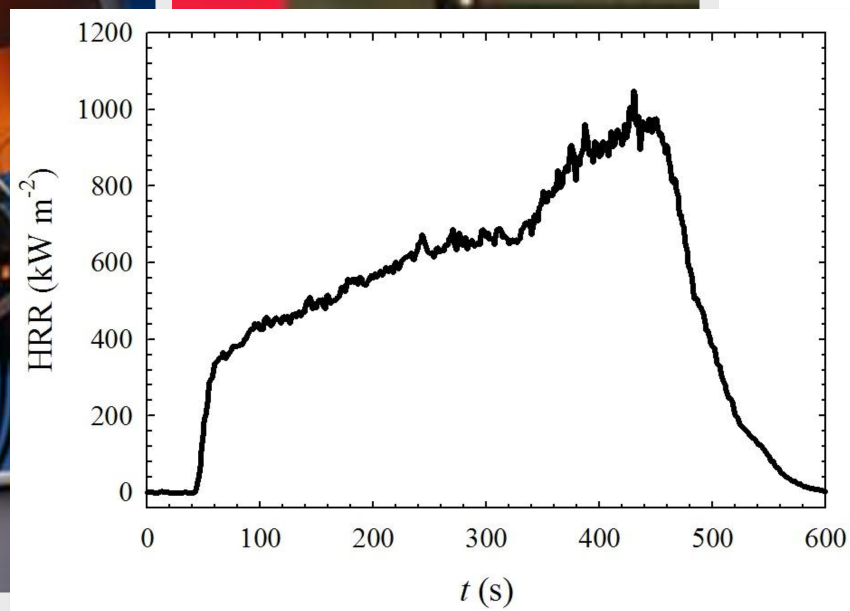
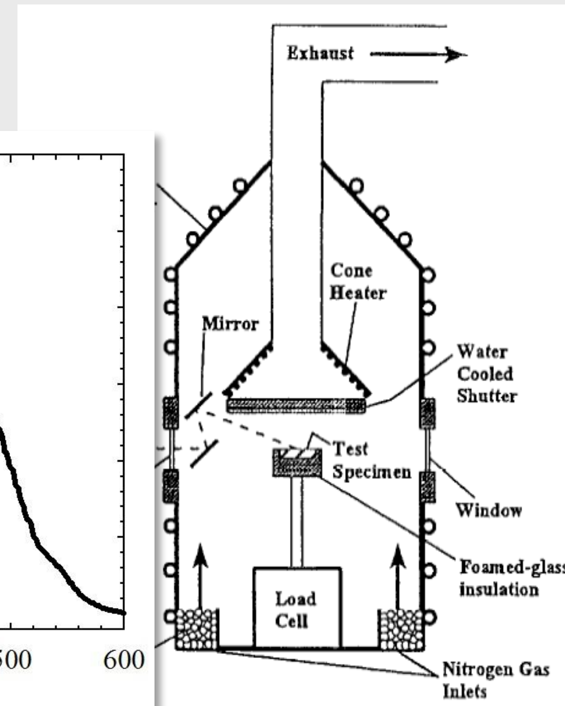


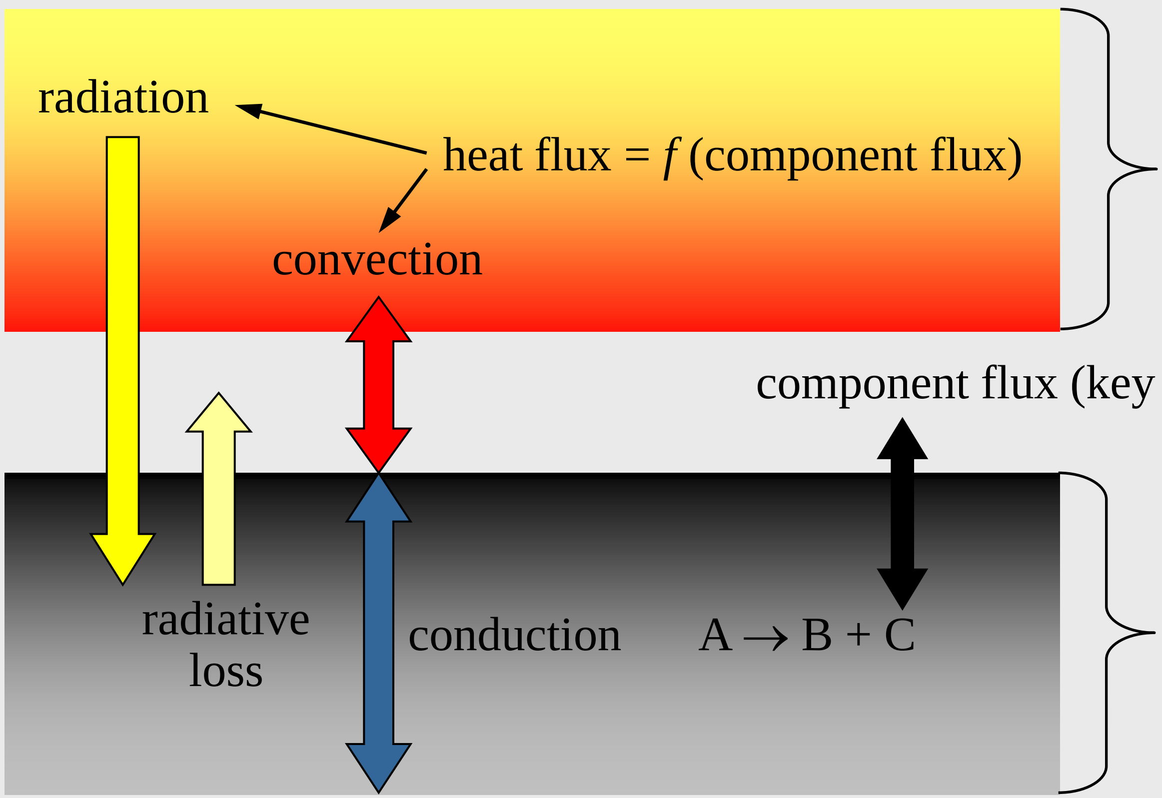
Fire Propagation Apparatus
(heat release measurement)



Gasification Apparatus
(mass loss measurement)



ThermaKin Model Overview



Gas phase is represented by empirical relations between heat flux and component fluxes. The relations are derived from experiments.

Condensed phase is represented by a mixture of components (A, B, C), which interact chemically and physically.

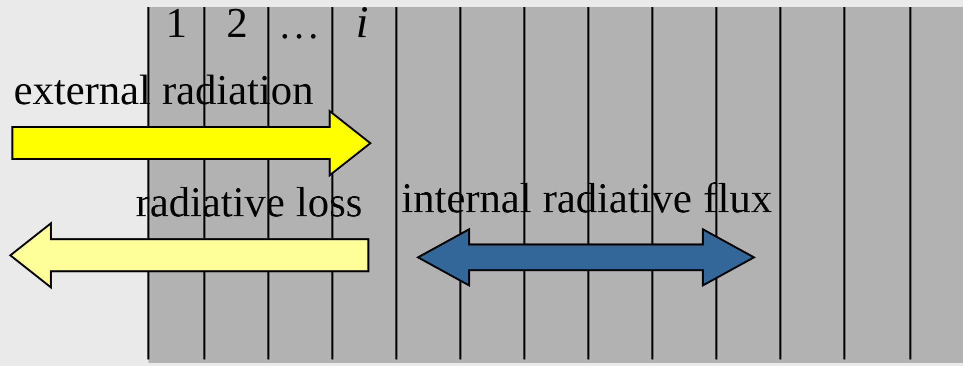
Radiative Energy Transfer

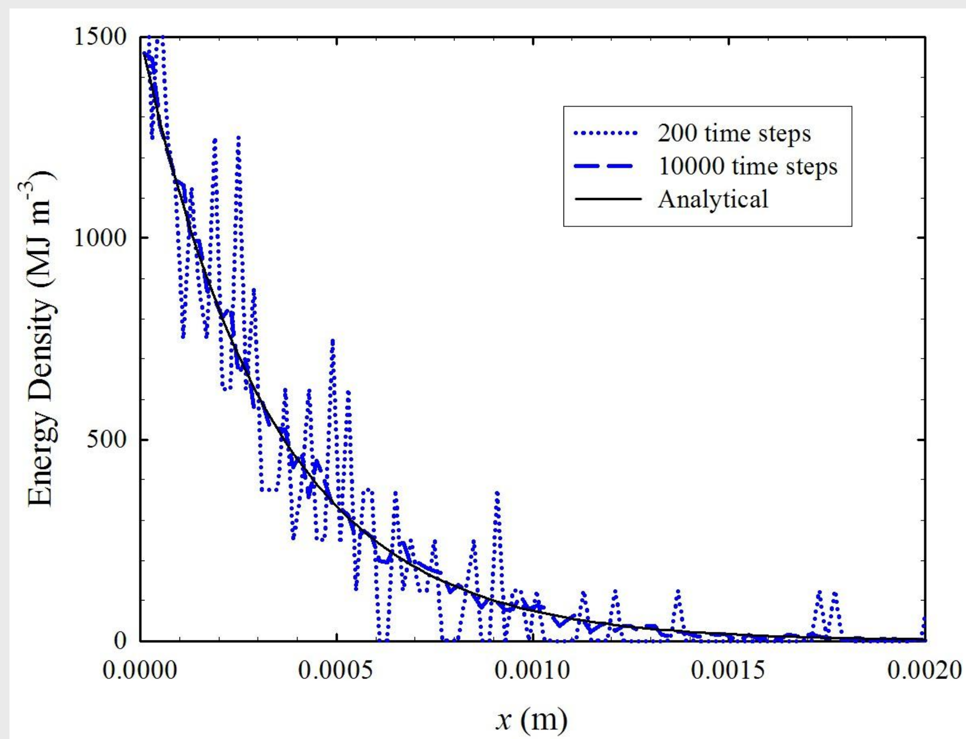
During any given time step, the external radiation is absorbed by a single element chosen at random.

$$\text{probability of absorption} = \frac{I_i \alpha_i \Delta x_i}{I_1}$$

$$\text{radiative loss} = \varepsilon_i \sigma T_i^4$$

$$\text{internal radiative flux} = -k_r \sigma T^3 \frac{\Delta T}{\Delta x}$$



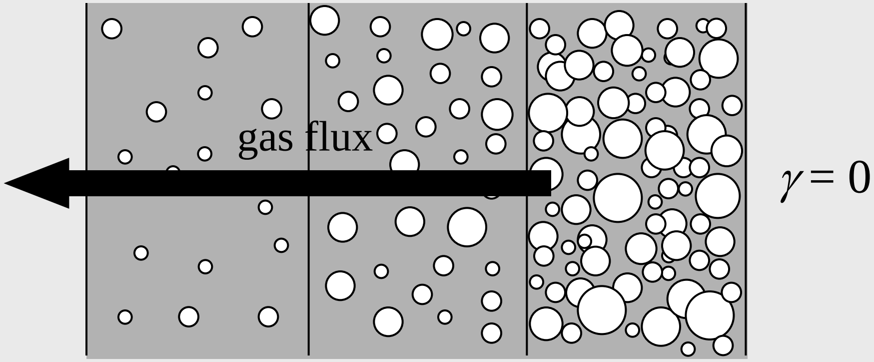


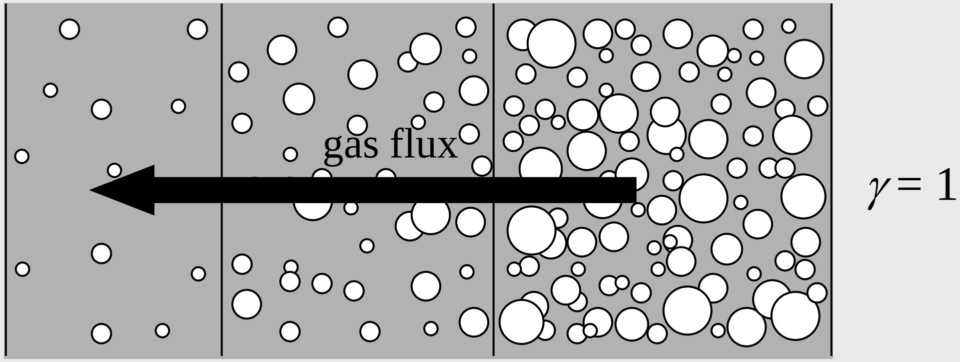
Mass Transfer

Components are categorized as solids, liquids, or gases.

$$\text{mass flux of gas} = -\lambda \rho_g \frac{\Delta\left(\frac{m_g / \rho_g}{V}\right)}{\Delta x}$$

Swelling factor γ defines volumetric reaction of the condensed phase to the presence of gases.



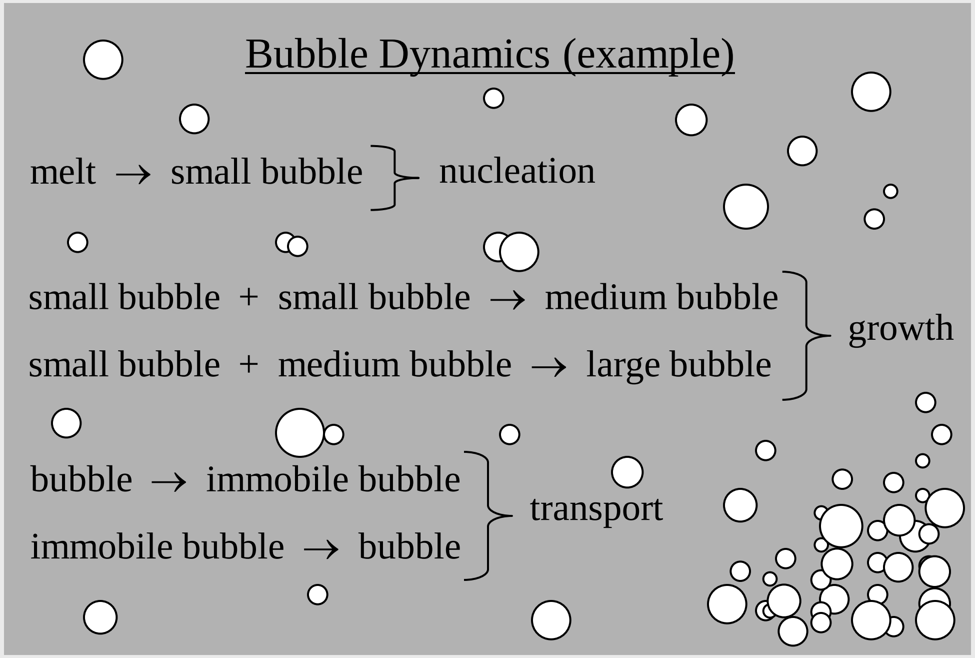


Chemical Reactions

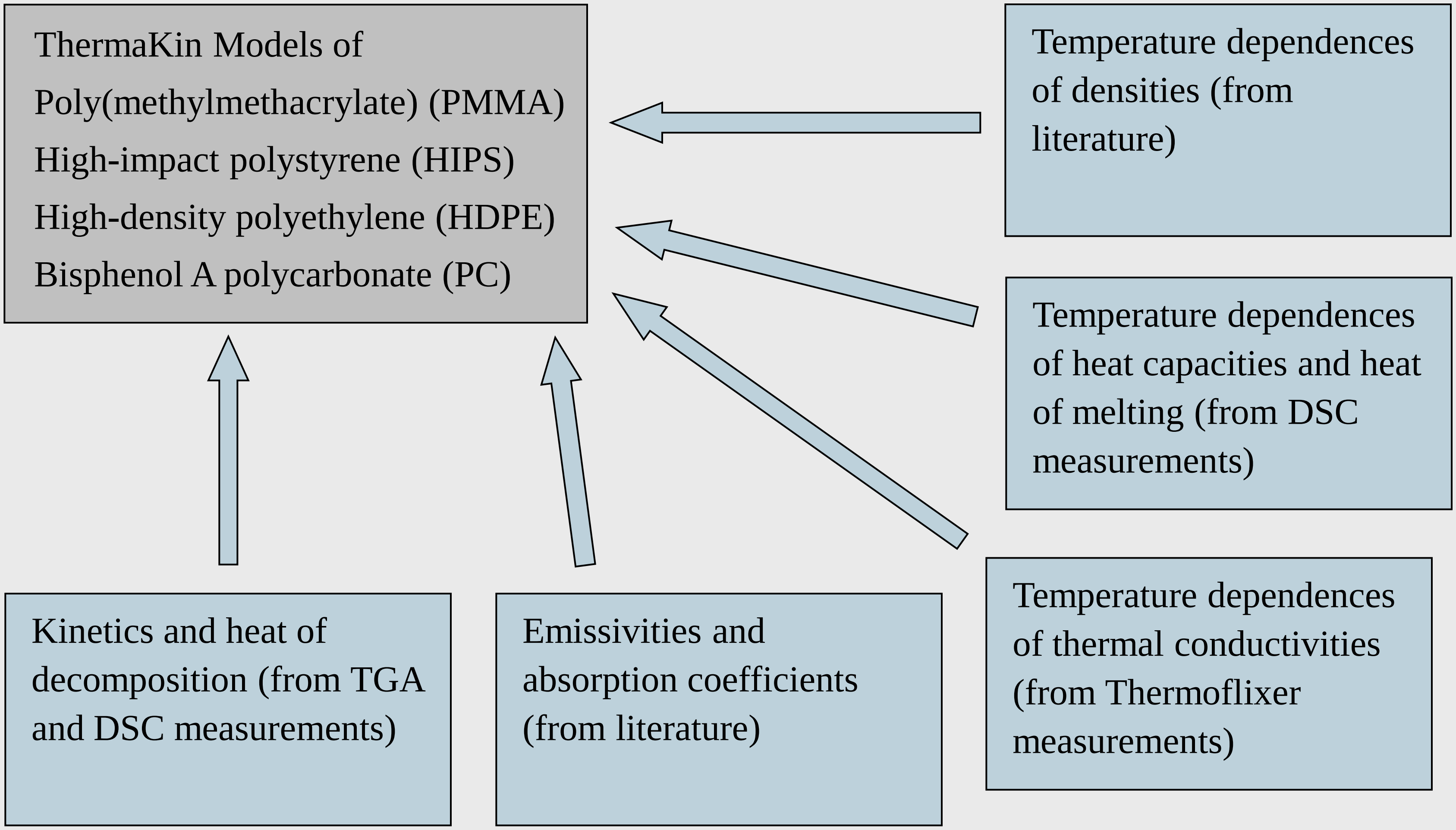
$$\theta_{\mathrm{A}}\,\mathrm{A} + \theta_{\mathrm{B}}\,\mathrm{B} \rightarrow \theta_{\mathrm{C}}\,\mathrm{C} + \theta_{\mathrm{D}}\,\mathrm{D} + \text{heat}$$

$$\text{rate} = \begin{cases} A\exp\left(-\dfrac{E}{RT}\right)\left[\dfrac{m_{\mathrm{A}}}{V}\right] \\ \qquad\qquad \text{or} \\ A\exp\left(-\dfrac{E}{RT}\right)\left[\dfrac{m_{\mathrm{A}}}{V}\right]\left[\dfrac{m_{\mathrm{B}}}{V}\right] \end{cases}$$

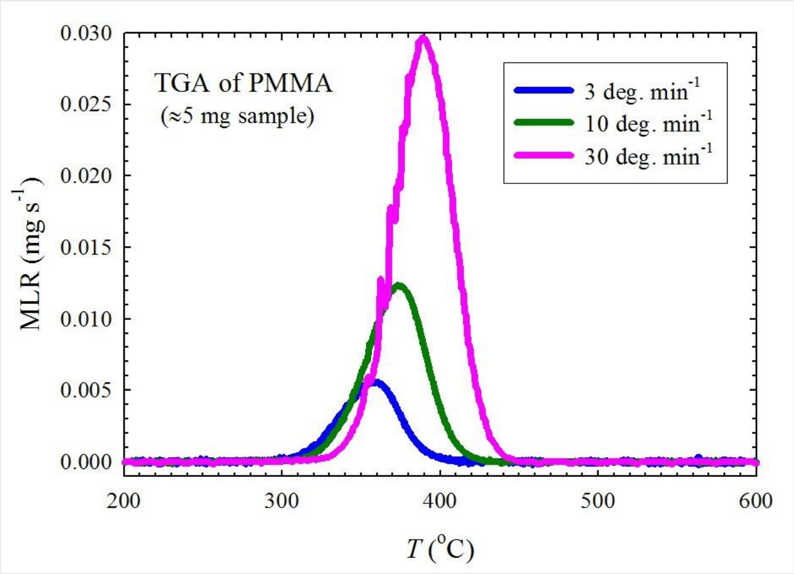
The reaction can be switched on or off at a specified temperature.



Parameterization



Kinetics of Decomposition

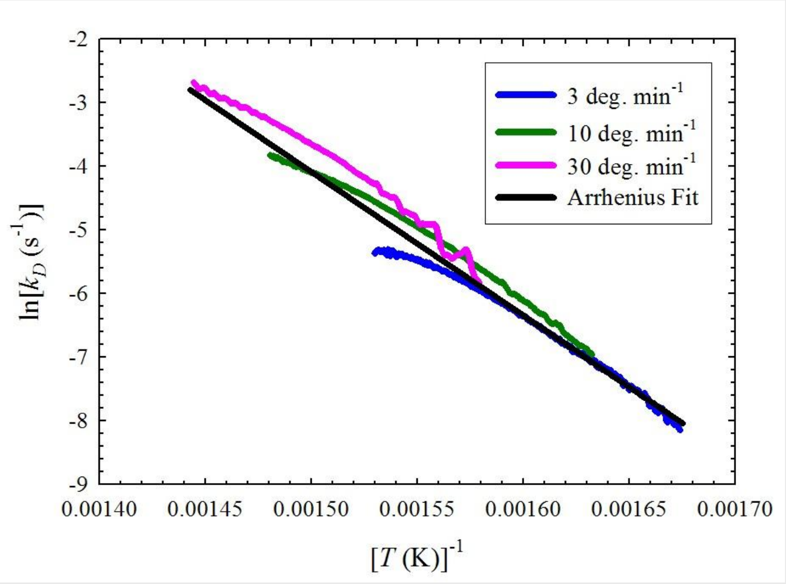


<u>Assumptions:</u>

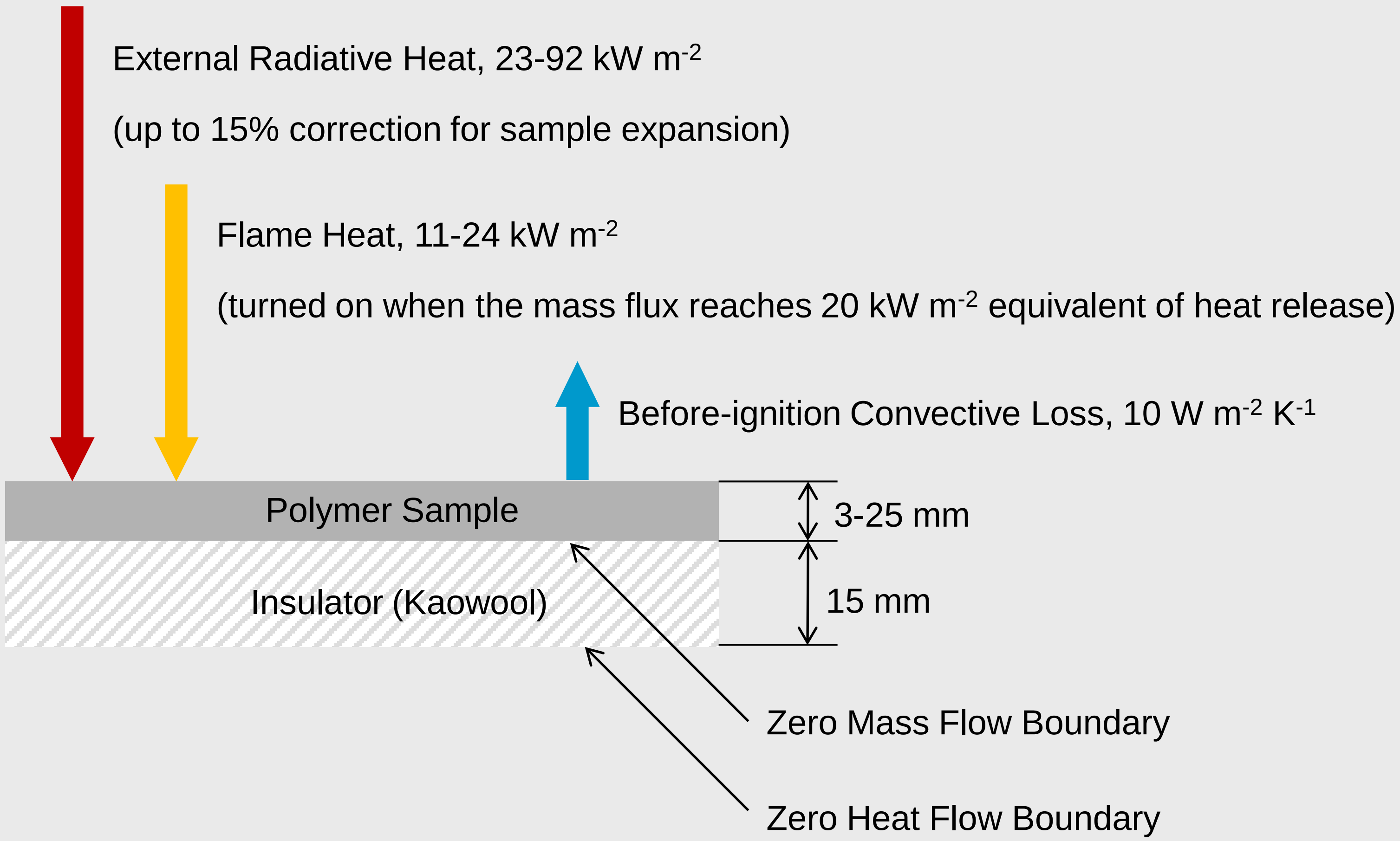
PMMA $\rightarrow$ Gas + heat

MLR = $k_D m_{\text{PMMA}}$ (first order)

Gas leaves PMMA instantaneously.



Modeling of Fire Calorimetry Experiments

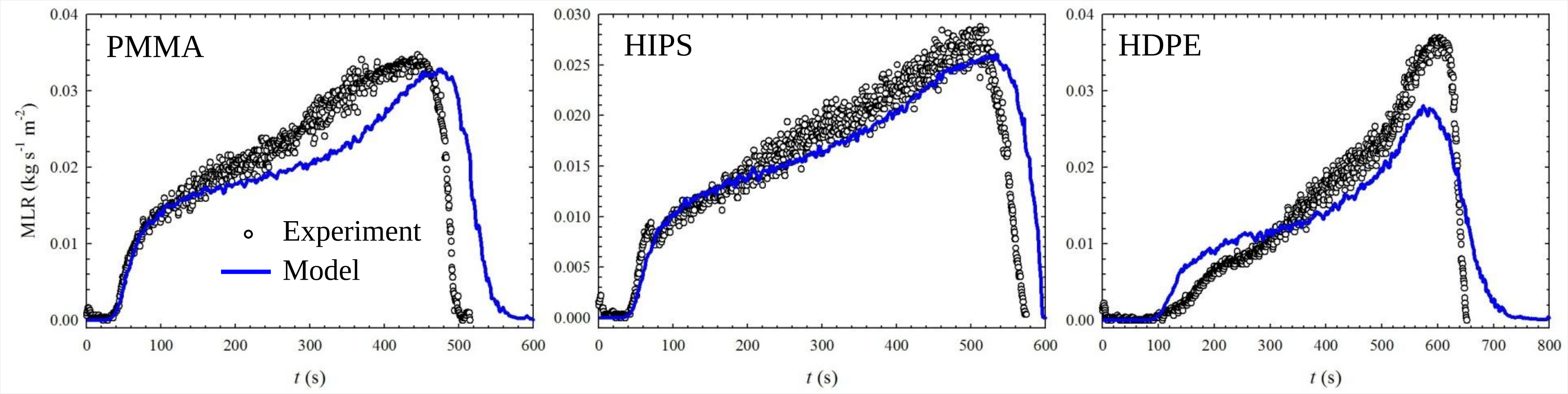


Gasification

Conditions:

external heat flux = 52 kW m^{-2}

initial sample thickness ≈ 9 mm

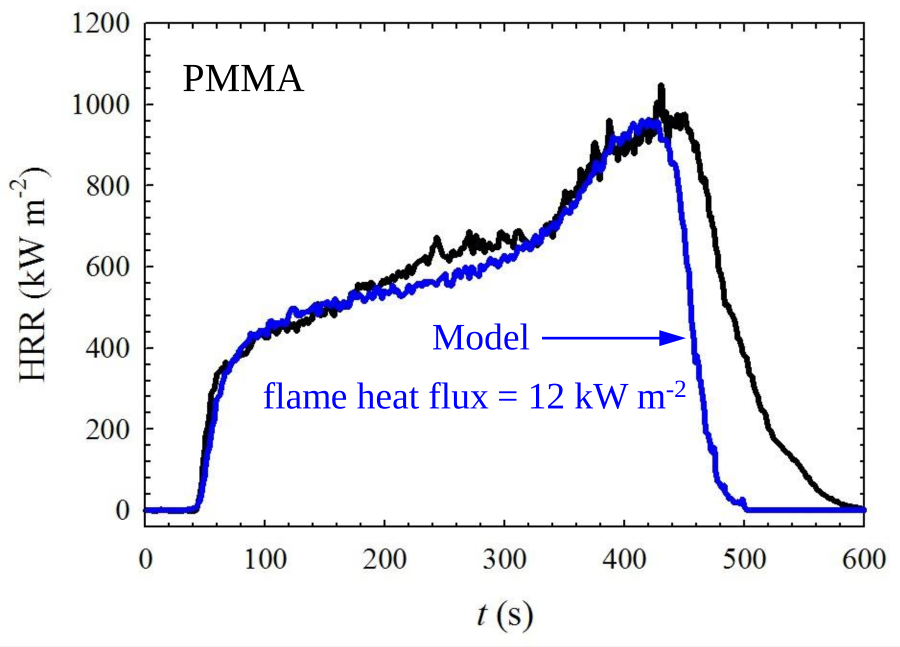


Cone Calorimetry

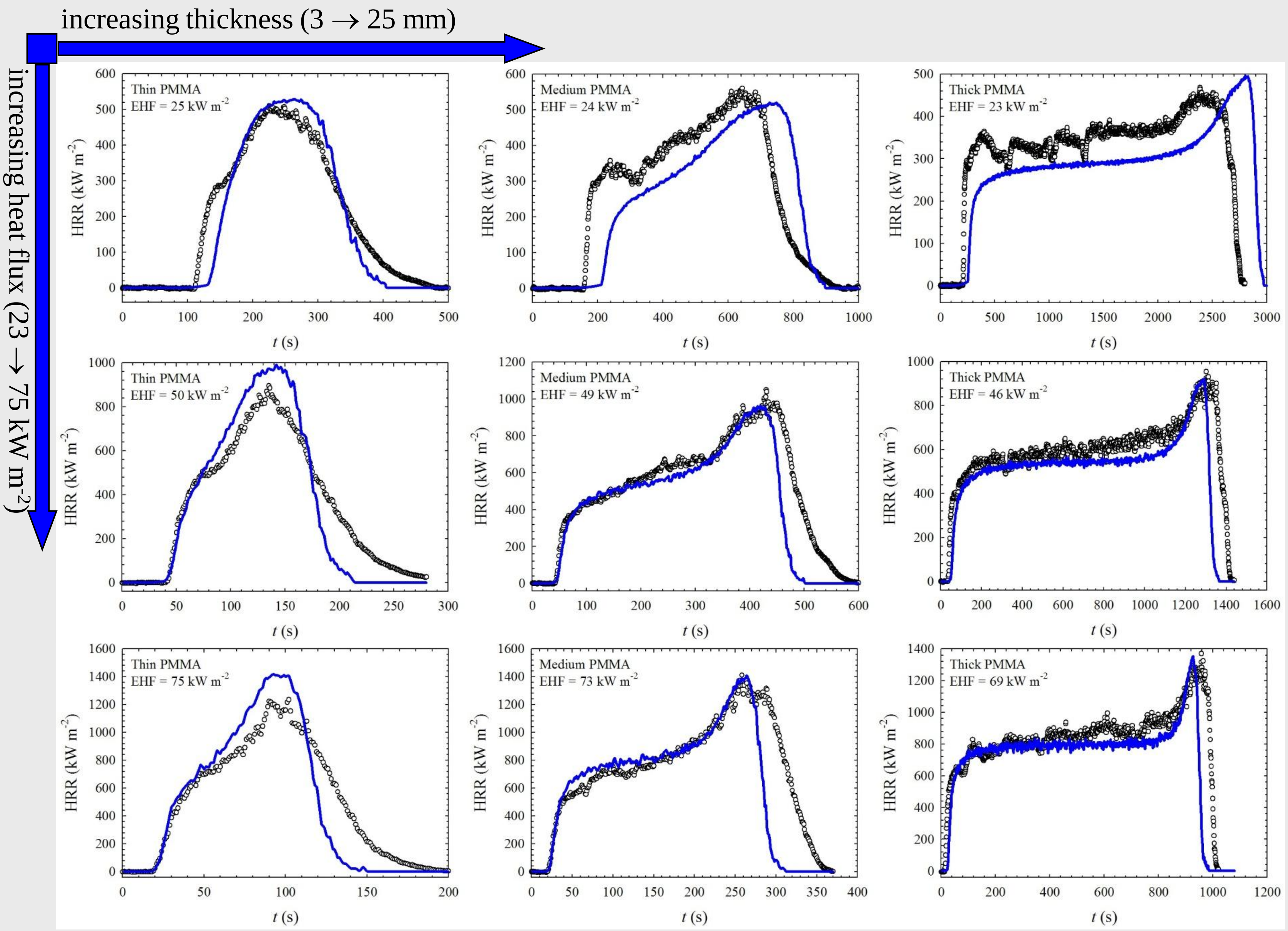
<u>Conditions:</u>

external heat flux = 49 kW m^{-2}

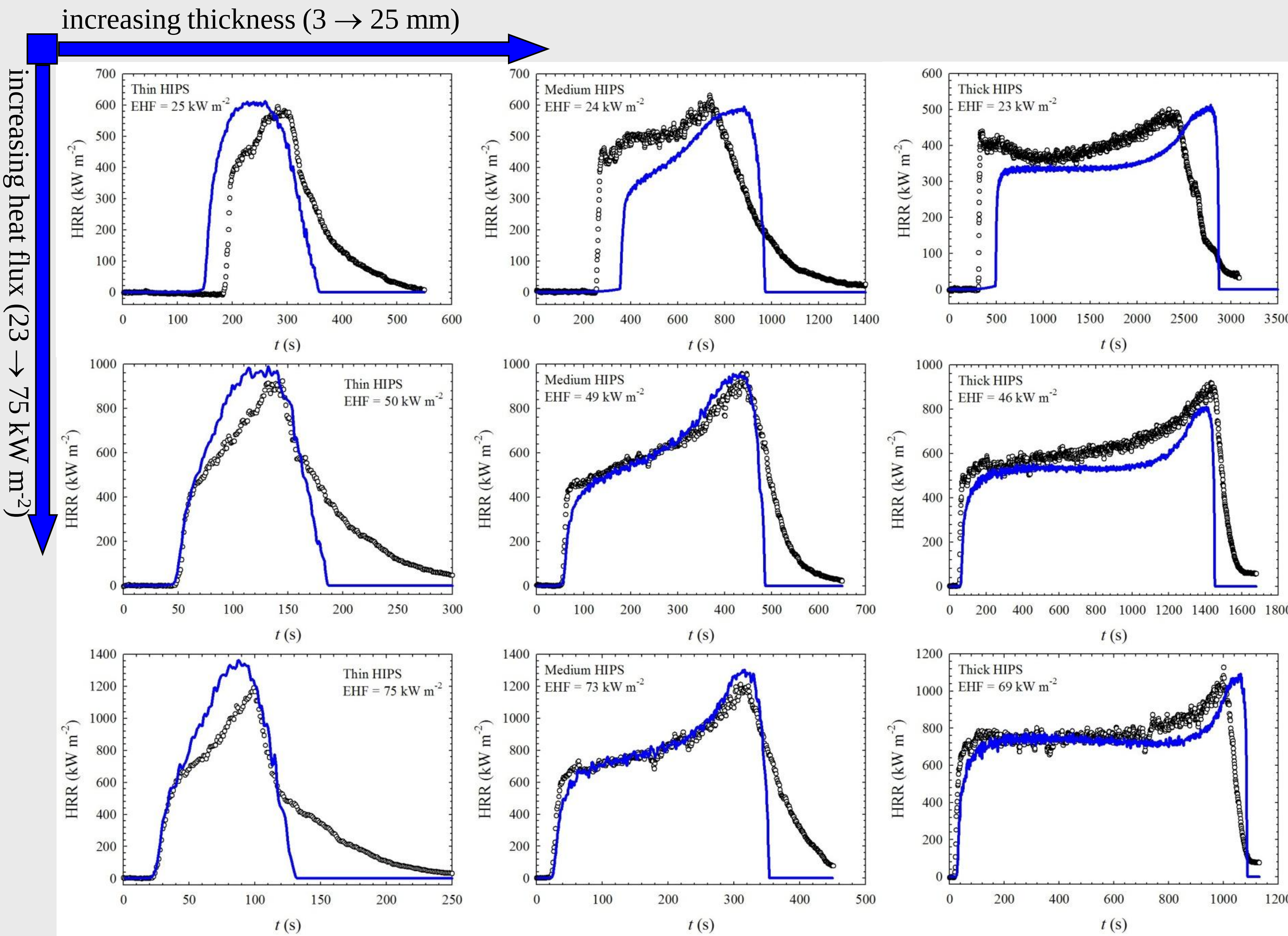
initial sample thickness ≈ 9 mm



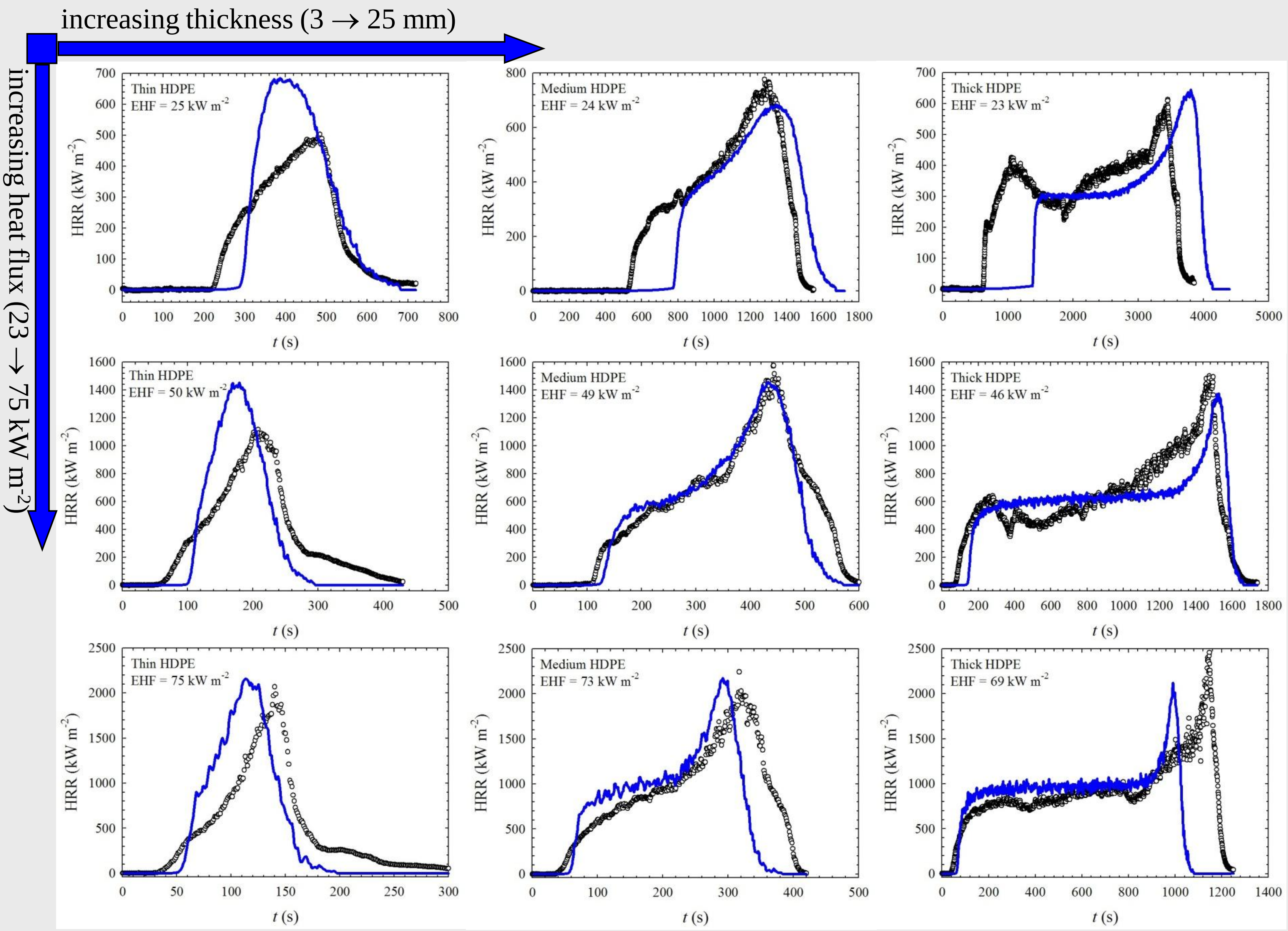
Cone Calorimetry of PMMA



Cone Calorimetry of HIPS



Cone Calorimetry of HDPE

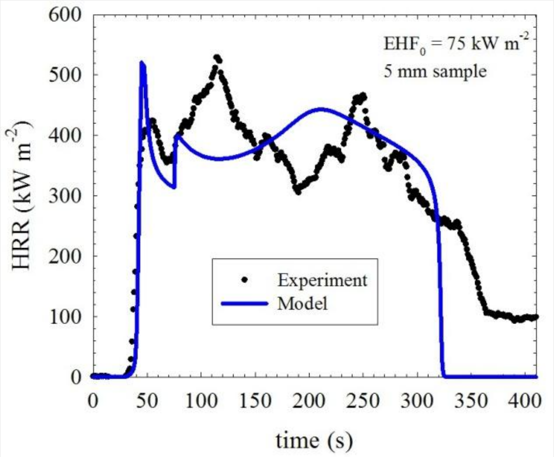


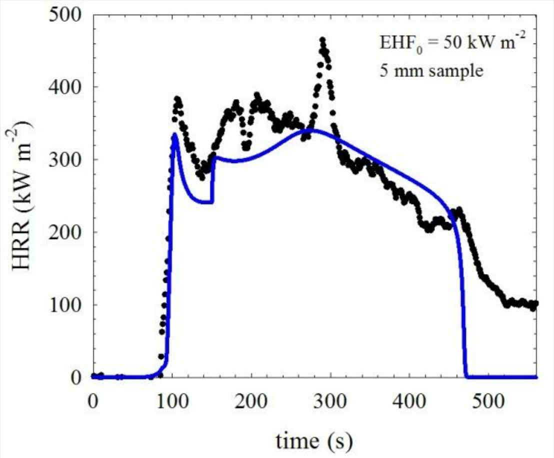
Cone Calorimetry of PC

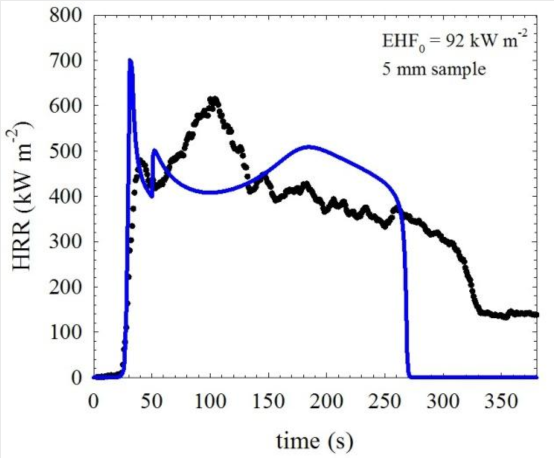
5 mm PC sample after 160 s at 75 kW m^{-2}.

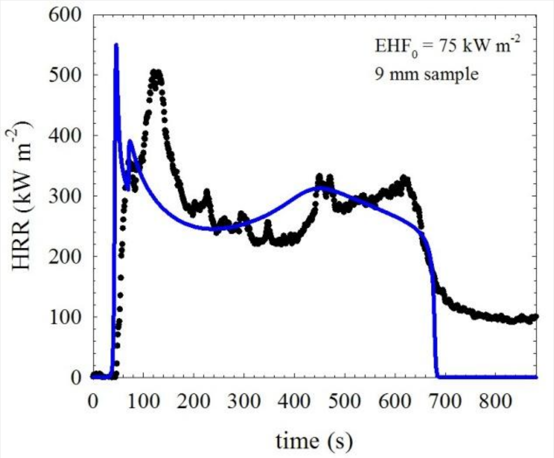
Flame heat flux = 15 kW m^{-2}.

The main mode of heat transfer inside char is radiation. The rate of transfer is defined by a single adjustable parameter.

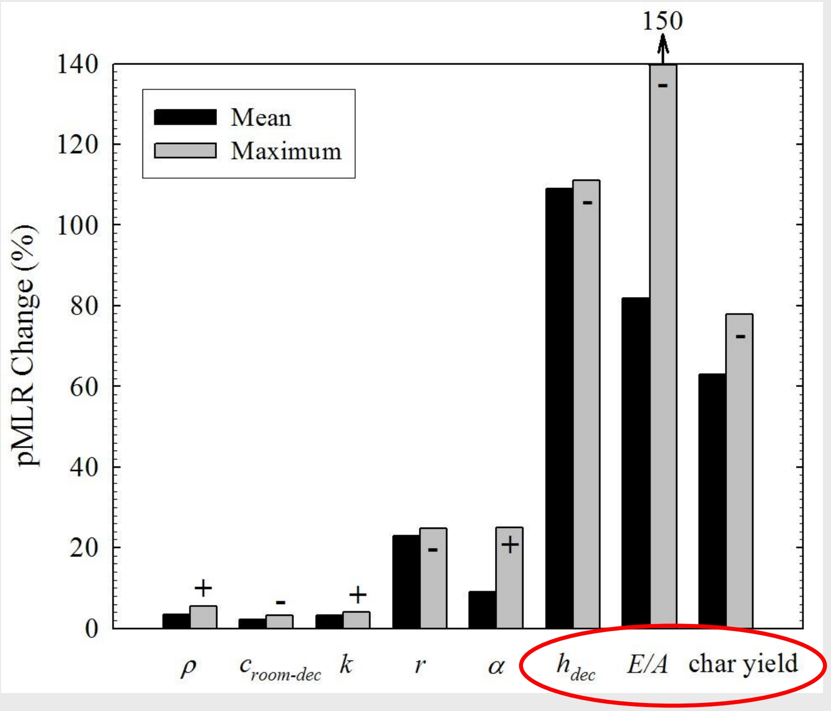


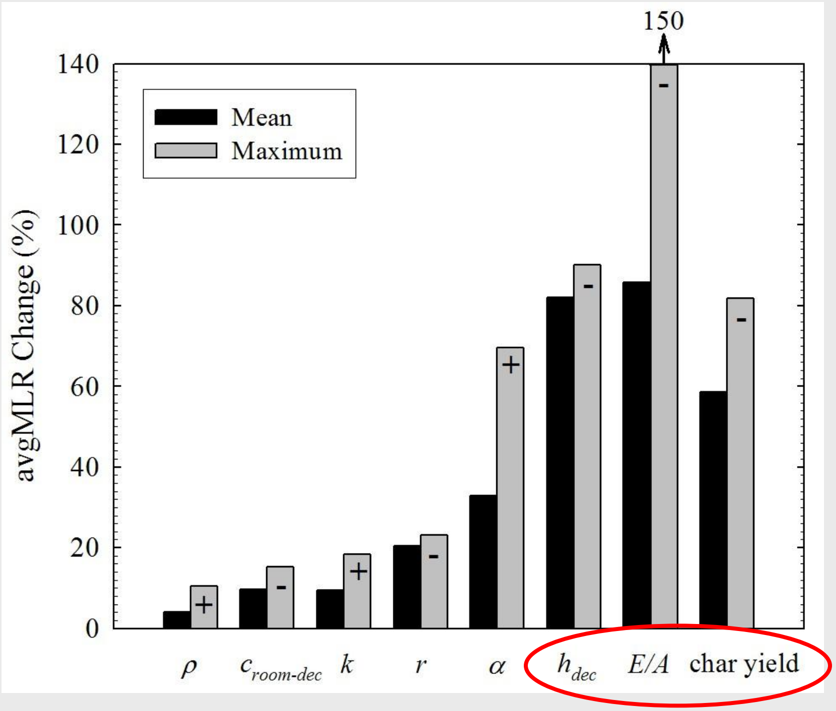






Sensitivity of Peak and Average Mass Loss Rates





Conclusions

- A one-dimensional numerical pyrolysis model can be used to predict the outcome of fire calorimetry experiments performed on polymeric materials.

- The predictions require the knowledge of chemical, thermal, and optical properties of the material. Measurement of these properties represents a challenging task.

- The rate of decomposition (defined by *A* and *E*), heat of decomposition, char yield and heat of combustion are the key parameters required for prediction of the peak and average heat release rates.